Non-Parametric Aerodynamic Shape Optimization

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Abstract. Numerical schemes for large scale shape optimization are considered. Exploiting the structure of shape optimization problems is shown to lead to very efficient optimization methods based on non-parametric surface gradients in Hadamard form. The resulting loss of regularity is treated using higher order shape Newton methods where the shape Hessians are studied using operator symbols. The application ranges from shape optimization of obstacles in an incompressible Navier–Stokes fluid to super- and transonic airfoil and wing optimizations.

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1. Introduction

1.1. Paradigms in Aerodynamic Shape Optimization

There are two paradigms to solve aerodynamic shape optimization problems: parametric and non-parametric. The non-parametric approach is traditionally used to derive analytically optimal shapes that can be globally represented as the graph of a function or by a deformation of the submanifold of the surface of the flow obstacle. With this paradigm, optimality of certain rotationally symmetric ogive shaped bodies in supersonic, irrotational, inviscid potential flows can be shown [15]. In the incompressible regime, optimal shapes for a viscous Stokes flow are derived in [20].

Any actual optimization so far follows the parametric paradigm. After choosing a finite dimensional design vector $q \in \mathbb{R}^{n_q}$, the gradient is computed by a formal Lagrangian approach:

$$\frac{df}{dq}(u(q), q) = \frac{\partial f}{\partial q} - \lambda^T \frac{\partial c}{\partial q},$$

where f is the objective function, u is the solution of the flow state $c(u,q)$, and λ is the adjoint variable. The mesh sensitivity Jacobian $\frac{\partial c}{\partial q}$ is a dense matrix. Often, the computation of the mesh sensitivity involves a mesh deformation procedure, making the computation of this Jacobian very costly. As the computational time and storage requirements increase quickly with the number of design parameters n_q, there is a strong desire to use as few design parameters as possible: Usually, the shape is deformed by a small number of smooth ansatz functions, where the coefficients of these functions are the design parameters. The de facto standard is a parameterization by Hicks-Henne functions [16], but sometimes b-spline parameters are also used.

Overcoming the limited search space of such a global parameterization in the form of coordinates of boundary points as design variables has long been desired, but the computational costs become prohibitive very quickly and the resulting loss of regularity is not well understood. A formulation of the gradient for the highly complex, nonlinear, hyperbolic equations describing compressible flows which can be computed without the design chain has long been sought after by both academia, [7] and [11], and industry [28, 29, 30, 31, 32]. More in line with the theoretical non-parametric approach, the problem is seldom treated from a true shape optimization perspective, except in [1, 2] for pressure tracking or in [4]. Due to the complexity of the shape differentiation techniques, none of the approaches above, which omit the design chain of the formal Lagrangian approach, have so far been successfully applied on a large scale drag reduction problem.

The work presented here follows mainly the non-parametric approach as a means to overcome the difficulties of the standard approach described above. Non-parametric shape gradients for various objectives and flow regimes will be discussed. Furthermore, shape Hessians can be exploited for convergence acceleration in higher order optimization approaches. The resulting shape-Newton methods define a new efficient algorithmic approach in aerodynamic non-parametric shape optimization. Such optimization problems are usually solved by a two loop approach: The outer loop is given by a gradient based optimization scheme, while solving the flow and adjoint equations creates the inner loop. This nested loop is rarely broken up, as in [14, 19] or in [13, 26]. The latter one-shot optimization relies on the structure of a standard non-linear finite dimensional optimization problem of the parametric approach [12]. Therefore, the need of a repeated mesh sensitivity computation usually reduces the effective speed-up for a large-scale shape parameterization. Therefore, similar to [23] a shape one-shot method is presented, which works outside the structure of a finite dimensional nonlinear problem and features a significant speed-up. As the standard approximation of the Hessian by BFGS-updates is questionable in this setting, we present a Hessian approximation based on operator symbols.

1.2. Shape Calculus

Shape calculus describes mathematical concepts when the geometry is the variable. Forsaking the shape problem origin by parameterizing, most—if not all—of the standard calculus of finite spaces is applicable. The alternative is to retain concepts of differential calculus, spaces of geometries, evolution equations, etc. to geometric domains. Excellent overviews about these concepts applied to shapes can be found in [6, 8, 27]. As both approaches are usually called "shape analysis", this field of research appears much more unified than it actually is. For example in the area of continuum mechanics and structural mechanics of elastic bodies the thickness of the material can be used to create a distributed parameter set. Alternatively, one can employ direct shape calculus techniques on the moving boundaries and topological derivatives in the interior [3, 5]. Outside of this compliance analysis, non-parametric shape calculus enables very elegant and efficient descriptions of sensitivities of general partial differential equations with respect to changes in the domain. However, there are many open questions when using these analytical objects numerically. For example, the proper discretization of analytic shape Hessians or finding reliable update formulas like BFGS need to be discussed more in order to better establish optimization schemes beyond shape gradient steepest descent. As such, higher order non-parametric shape optimization schemes are rare. In [9] the shape Hessian is studied via sinusoidal perturbations of the annulus, in [10] the shape Hessian for potential flow pressure tracking in star-shaped domains is considered, and in [17, 18] a non-parameterized image segmentation approach is shown, also employing shape Hessians.

2. Impulse Response Approach for Characterizing Shape Hessians in Stokes and Navier–Stokes Flow

The research presented in this section focuses on finding reliable and easily applicable shape Hessian approximations for flow problems governed by the incompressible Navier–Stokes equations. We study shapes that minimize the conversion of kinetic energy into heat, which is physically closely related to a proper drag reduction using the formulation based on surface forces. The model problem for finding shape Hessians is given by:

$$\min_{(u,p,\Omega)} J(u,\Omega) := \int_\Omega \nu \sum_{i,j=1}^{3} \left(\frac{\partial u_i}{\partial x_j}\right)^2 \, dA \tag{2.1}$$

$$\begin{aligned} \text{s.t.} \; -\nu\Delta u + \rho u \nabla u + \nabla p &= 0 \quad \text{in} \quad \Omega \\ \operatorname{div} u &= 0 \\ u &= 0 \quad \text{on} \quad \Gamma_1 \qquad (2.2) \\ u &= u_\infty \quad \text{on} \quad \Gamma_2 \\ \text{Volume}(\Omega) &= V_0, \end{aligned}$$

where $u = (u_1, u_2)^T$ is the speed of the fluid, ν is the kinematic viscosity, p denotes the pressure, and ρ is the density which is constant in an incompressible fluid. Also, $\Gamma_1 \subset \partial\Omega$, the no-slip surface of the flow obstacle, is the unknown to be found. The shape derivative for this problem is given by:

$$dJ(u,\Omega)[V] = \int_\Gamma \langle V,n\rangle \left[-\nu \sum_{k=1}^{3} \left(\frac{\partial u_k}{\partial n}\right)^2 - \frac{\partial u_k}{\partial n}\frac{\partial \lambda_k}{\partial n}\right] \, dS,$$

where $\lambda = (\lambda_1, \lambda_2)^T$ and λ_p again satisfy the adjoint equation

$$\begin{aligned} -\nu\Delta\lambda - \rho\lambda\nabla u - \rho\left(\nabla\lambda\right)^T u + \nabla\lambda_p &= -2\Delta u \quad \text{in } \Omega \\ \text{div } \lambda_p &= 0 \qquad\quad \text{in } \Omega. \end{aligned}$$

For more details see [22, 24, 25]. The idea is to characterize the Hessian of this problem by its symbol, which is defined as the image of a single fourier mode $\tilde{q}(x) := \hat{q}e^{i\omega x}$ under the Hessian H of the problem.

If we assume $\Omega = \{(x,y) : x \in \mathbb{R}, y > 0\}$ to be the upper half-plane, then we need to track the Fourier mode $\alpha(x) := e^{i\omega_1 x}$ through the perturbation of the local shape derivatives

$$\begin{aligned} u_i'[\alpha] &= \hat{u}_i e^{i\omega_1 x} e^{\omega_2 y} \\ p'[\alpha] &= \hat{p} e^{i\omega_1 x} e^{\omega_2 y}. \end{aligned} \tag{2.3}$$

In the limit of the Stokes case, $\rho = 0$, the perturbed shape gradient $dG_\Gamma[\alpha]$ is given by

$$dG_\Gamma[\alpha] = -2\nu \sum_{i=1}^{2} \frac{\partial u_i}{\partial y}\frac{\partial u_i'[\alpha]}{\partial y},$$

which means that the Hessian H is defined by the mapping

$$\frac{\partial u_i'[\alpha]}{\partial y} = H\alpha.$$

Thus, if the angular frequency ω_1 can be made explicit in the left hand side, we

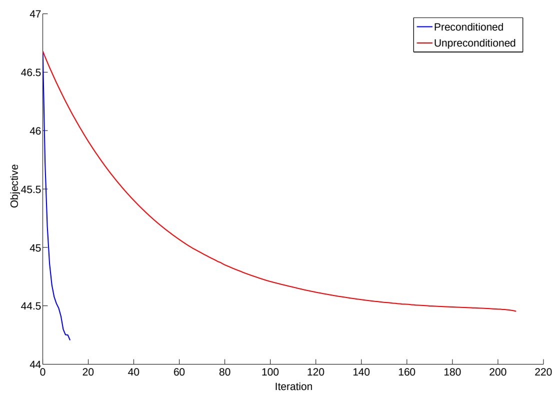

FIGURE 1. Preconditioning accelerates the Stokes problem by 96%.

have exactly the definition of the operator symbol as stated above. To achieve this, the PDE defining the local shape derivatives is transformed into the Fourier space. There, the solvability requirement of the PDE and its boundary conditions in the frequency space defines an implicit function relating ω_2 to ω_1 in (2.3). Essentially, this implicit function is given by the roots of the characteristic polynomial of the PDE for the local shape derivatives and gives for the Stokes problem:

$$\det dC[\alpha] = \nu(-\omega_1^2 + \omega_2^2)\omega_2^2 - \nu(-\omega_1^2 + \omega_2^2)\omega_1^2. \tag{2.4}$$

Using this method, one can show that the shape Hessian for the Stokes problem is a pseudo-differential operator of order $+1$, closely related to the Poincaré-Stecklov operator. The task of identifying the shape Hessian is thus transformed to finding an explicit representation of a certain implicit function in the Fourier space.

Finding explicit representations of implicit functions analytically is still infeasible for more complex problems. For an empirical determination of the symbol

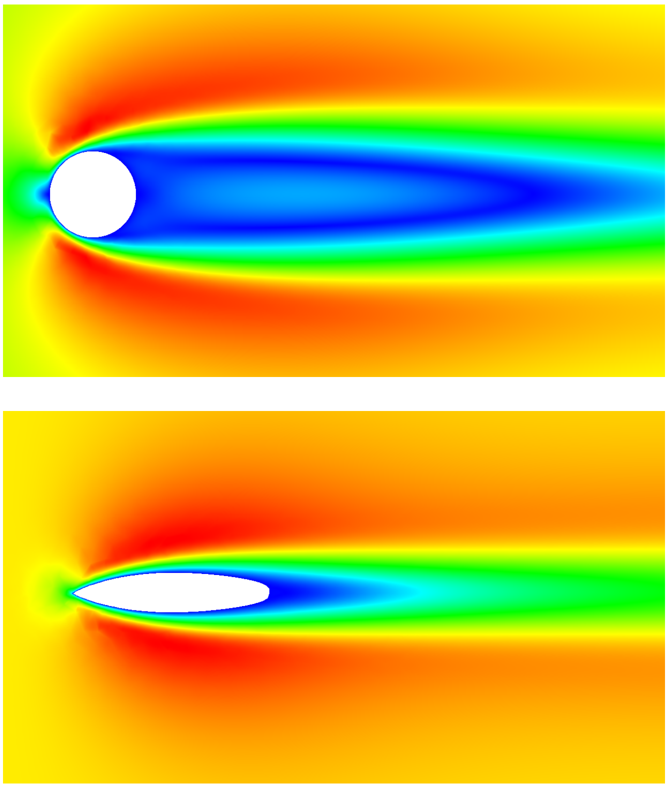

Figure 2. Initial and optimized Navier-Stokes shapes. Color denotes speed.

of the Navier–Stokes shape Hessian see [22, 24], where the operator is found to be a pseudo-differential operator with the symbol $|\omega|$, again closely related to the

Poincaré-Stecklov operator. We approximate this operator by a damped Laplace-Beltrami operator for preconditioning these problems, where the damping is determined by the frequency spectrum of the standing waves possible on the given mesh resolution of the surface. This leads to a significant speed-up of 96% in the Stokes case and of 80% in the Navier-Stokes case. The speed-up for the Stokes case is shown in figure 1 and the initial and optimal shapes for the Navier–Stokes problem can be seen in figure 2: The double vortex behind the initial circle has been completely removed.

3. Exploitation of Shape Calculus for Supersonic and Transonic Euler Flow

3.1. Introduction

As the usual cruise speed is Mach 0.7 and more, the incompressible Navier–Stokes equations considered above are not a sophisticated enough flow model: viscosity effects become negligible compared to compression effects, which means that we must now at least consider the compressible Euler equations as a model for the flow. At transonic and supersonic flow conditions, shock waves form that dominate the drag of the aircraft. This means not only that the discontinuous solutions must be computed correctly for the forward and adjoint problem, but also that the shape derivative must give correct results under a PDE constraint which has a discontinuous solution. We found that the nodal shape-Newton method works very well given a discontinuous state. The objective function is now a proper force minimization and the whole drag optimization problem is stated as:

$$\begin{aligned}
\min_{(U,\Omega)} F_{\text{drag}}(U,\Omega) \quad &:= \quad \int_\Gamma \langle p_d, n\rangle \; dS \\
\text{s.t.} \sum_{i=1}^{3} A_i(U_p)\frac{\partial U}{\partial x_i} \quad &= \quad 0 \text{ in } \Omega \text{ (Euler equations)} \\
\langle u, n\rangle \quad &= \quad 0 \text{ on } \Gamma \text{ (Euler slip condition)} \\
F_{\text{lift}}(U,\Omega) := \int_\Gamma \langle p_l, n\rangle \; dS \quad &\geq \quad l_0 \text{ (lift force)} \\
L := \int_\Gamma dS \quad &\leq \quad L_0 \text{ (airfoil contour length)} \\
I_x := \int_\Gamma (y-y_c)^2 \, dS \quad &\geq \quad I_{x_0} \text{ (airfoil bending stiffness).}
\end{aligned}$$

For 2D applications there is also the additional constraint that the leading edge is fixed at $(0,0)^T$ and the trailing edge must be fixed at $(1,0)^T$. Otherwise, the optimization changes the reference length of the airfoil, which would lead to a wrong non-dimensionalization of the flow quantities. The contour length constraint and bending stiffness constraint are usually not engaged at the same time. They are both not very sophisticated and serve as a substitute for a proper modeling of the airfoil's structure. Without them, the solution will either degenerate into a flat line or will not be of any practical relevance.

Additionally, $U := (\rho, \rho u_1, \rho u_2, \rho u_3, \rho E)^T$ is the vector of the unknown state and denotes the conserved variables, where ρ is the density of the fluid, u_i are the velocity components, and E is the internal energy of the fluid. Likewise, $U_p := (\rho, u_1, u_2, u_3, E)^T$ denotes the primitive variables which enter the Euler flux Jacobians $A_i := \frac{\partial F_i}{\partial U}$ of the inviscid fluxes F_i. Using the non-conservative formulation of the Euler equations in terms of the flux Jacobians simplifies the derivation of the adjoint equations. For a given angle of attack α, we define $p_d := p \cdot (\cos\alpha, \sin\alpha)^T$ and $p_l := p \cdot (-\sin\alpha, \cos\alpha)^T$, where p denotes the pressure, which is related to the conserved variables by the perfect gas law $p = (\gamma - 1)\rho(E - \frac{1}{2}(u_1^2 + u_2^2 + u_3^2))$. Here, γ is the isentropic expansion factor, i.e. the heat capacity ratio, of air. For the bending stiffness constraint, y is the y-coordinate of the contour, and y_c is the y-coordinate of the center of mass of the contour.

The numerous mappings of the pressure p to the conserved variables U makes the derivation of the shape derivative non-trivial. In fact, the shape derivative for this problem was long sought after for the benefits stated above. In the engineering literature often called "surface formulation of the gradient", there have been previous attempts to find the shape derivative [4, 7, 11, 28] The surface measure variation dS_ϵ must be considered, because a boundary integral objective function requires a partial integration on the surface of submanifolds, which usually introduces additional curvature terms. Considering this, the shape derivative of the Euler drag reduction is given by

$$\begin{aligned} dF_{\text{drag}}(\Omega)[V] &= \int\limits_\Gamma \langle V, n\rangle \left[\langle \nabla p_d\, n, n\rangle + \kappa\langle p_d, n\rangle\right] + (p_d - \lambda U_H u) dn[V]\; dS \qquad (3.1)\\ &= \int\limits_\Gamma \langle V, n\rangle \left[\langle \nabla p_d\, n, n\rangle + \operatorname{div}_\Gamma(p_d - \lambda U_H u)\right]\; dS, \end{aligned}$$

where λ solves the adjoint Euler equations:

$$-A_1^T \frac{\partial}{\partial x_1}\lambda - A_2^T \frac{\partial}{\partial x_2}\lambda - A_3^T \frac{\partial}{\partial x_3}\lambda = 0 \text{ in } \Omega$$

and the wall boundary condition

$$(\lambda_2, \lambda_3, \lambda_4)\, n + n_d = 0$$

on the wing. Here, $U_H := (\rho, \rho u_1, \rho u_2, \rho u_3, \rho H)^T$ are the conserved variables with the last component replaced by the enthalpy $\rho H = \rho E + p$. Also, $\operatorname{div}_\Gamma$ denotes the divergence in the tangent space of Γ, which is sometimes also called "surface divergence". Also, κ denotes additive mean curvature. Thus, a correct computation of the shape derivative also requires discrete differential geometry, as the curvature and normal variation or surface divergence must be computed correctly on the given CFD mesh.

The following results were achieved with the DLR flow solver TAU, which is an unstructured finite volume code, in Euler mode. It features an implementation of the continuous adjoint and is also the production code of Airbus, making the following computations examples of real world applications. The Hessian is a pseudo-differential operator of order +2. For the smoothing procedure we always employed the Laplace-Beltrami operator.

3.2. Supersonic Airfoil Optimization

The first test was conducted for a fully supersonic flow at no angle of attack and no lift constraint. The fully supersonic case is considered easier, because the initial NACA0012 airfoil produces a detached bow shock due to its blunt nose. Thus, the state is continuous where the shape derivative must be evaluated. The

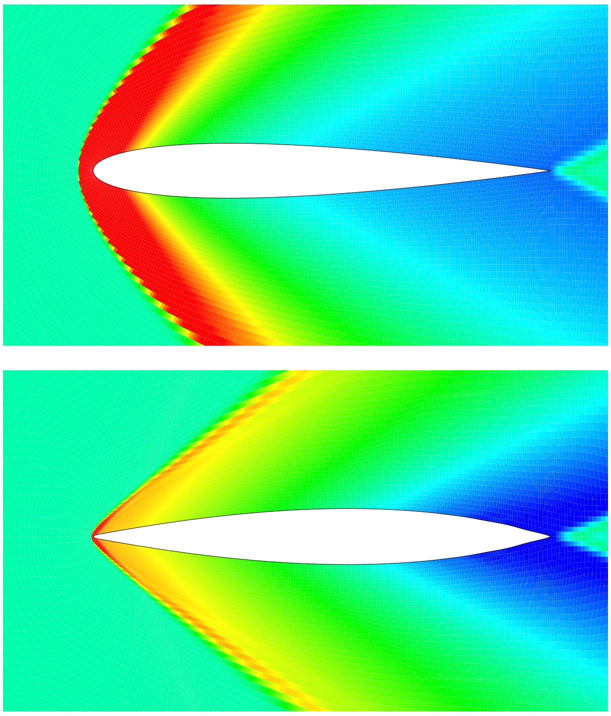

FIGURE 3. Non-lifting optimization, supersonic flow Mach 2.0. NACA0012 airfoil deforms to a Haack Ogive shape. Color denotes pressure.

shapes can be seen in figure 3. We have the automatic formation of a sharp leading edge without user intervention. The strong detached bow shock of the blunt nose

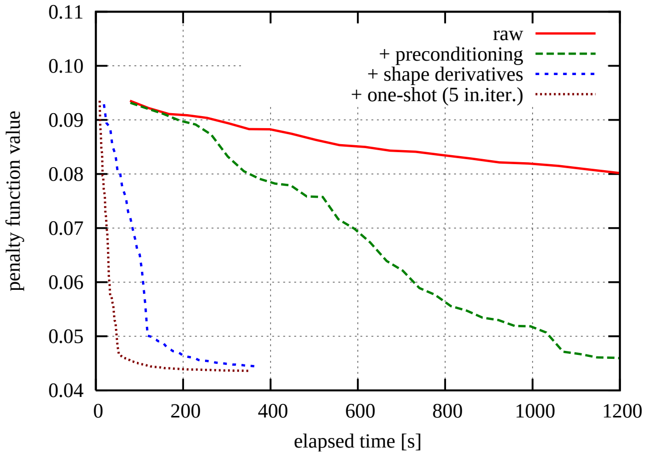

FIGURE 4. Speed-up in CPU time due to shape Hessian preconditioning, shape derivative, and one-shot.

body is transformed to a weaker attached shock of a body with a sharp leading edge. The optimal shape, a Haack Ogive, was expected from the literature, as it is analytically known from simpler supersonic inviscid flow models that such shapes are optimal, making this an excellent test to gauge the method against. The correct shape was very efficiently found: From an initial $C_D = 9.430 \cdot 10^{-2}$, the optimal $C_D = 4.721 \cdot 10^{-2}$ was found with 2.5 times the cost of the simulation alone. Using the shape Hessian, the shape derivative, and a one-shot approach, we can solve this problem in about 100 seconds. The classical approach of solving a non-linear optimization problem post discretization requires 2.77 hours. The CPU time reduction of one-shot, shape derivative, and shape Hessian are all cumulative, making the nodal one-shot approach 99% faster. The effects of each ingredient can be seen in figure 4.

3.3. Onera M6 Wing Optimization

We conclude with the optimization of the Onera M6 wing in three dimensions. During cruise condition of Mach 0.83 and 3.01° angle of attack, the wing features a lift coefficient of $C_L = 2.761 \cdot 10^{-1}$ and a drag coefficient of $C_D = 1.057 \cdot 10^{-2}$. This drag is mainly created due to two interacting shock waves on the upper side of the wing. Thus, in this three dimensional application, the wing shape must be optimized such that the shock waves vanish while at the same time maintaining lift and internal volume, which adds another constrained compared to the problem considered above. We conduct a multi-level optimization using all CFD mesh surface nodes as design parameter. The coarse mesh features 18,285 surface nodes and a finer mesh is created adaptively during the optimization with has 36,806 surface nodes. Surface finite elements in a curved space are used to compute the

Laplace–Beltrami operator for the Hessian approximation. Likewise, the curvature is computed by discretely constructing the second fundamental tensor **II** similar to [21]. The resulting optimal shapes are shown in figure 5. The optimized wing

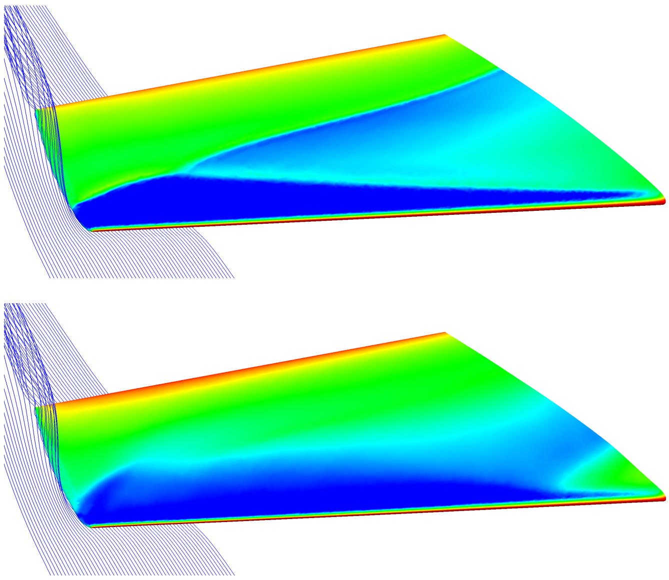

FIGURE 5. Initial and optimized Onera M6 wing. Color denotes pressure. The upper surface shock waves are completely removed.

is shock free with a drag coefficient of $C_D = 7.27 \cdot 10^{-3}$ and maintains lift with $C_L = 2.65 \cdot 10^{-1}$.

4. Conclusions

Large scale aerodynamic shape optimization was considered. While usually the actual computation of optimal shapes is based on a parametric approach, here we focus on a non-parametric shape sensitivity analysis in order to very efficiently compute the shape gradients. Paired with a one-shot optimization approach, this creates a highly efficient numerical scheme exploiting the nature of shape optimization problems, e.g. the possibility of computing the gradient using surface quantities alone. The resulting loss of regularity is treated using higher order optimization methods where the shape Hessian is approximated using operator symbols. Both the incompressible Navier–Stokes equations as well as the compressible Euler equations are considered as a model for the fluid and both the shape optimization of obstacles in a flow channel as well as super- and transsonic airfoil and wing optimizations are presented.

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